Travis Sjostrom

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Education

2002–2008	Department of Physics, University of Utah, graduate student. Specialization in condensed matter theory and computation. Thesis - "Electronic Energy Band Calculations in Nano-structures" Supervisor - Daniel C. Mattis Graduated 2008, Ph.D.
1997-2002	University of Utah, undergraduate student. Graduated 2002, B.S. Physics.

Experience & Skills

Feb 2016-Present	Staff Scientist, Theoretical Division, T-1, Los Alamos National Laboratory Development and application of quantum molecular dynamics, including orbital-free DFT, for equation of state of materials. Further development on the underlying modeling and code used for equation of state generation.
2013-Feb 2016	Postdoctoral Associate, Theoretical Division, T-5, Los Alamos National Laboratory Orbital-free DFT theory and code development for molecular dynamics simulations and average atom models, including time-dependent orbital-free and beyond Born-Oppenheimer formulations. Applications to equation of state of materials.
2009-2012	Postdoctoral Associate, Quantum Theory Project, University of Florida Research and development of DFT methods for warm dense matter, including exchange-correlation and orbital-free kinetic energy functionals, and pseudopotentials. Ran and modified various DFT programs, wrote MPI thermal *ab initio* and DFT programs, established and maintained group website.
2004–2008	Research Assistant, University of Utah Thesis - "Electronic Energy Band Calculations in Nano-structures:" Density functional theory calculations for a semiconducting quasi-2D antidot nano-array, as high temperature superconductor model, finding different magnetic ground state depending on geometry and also on an electron filling factor. 2D Hubbard and t-J model comparisons on small clusters.
Jun 2005–Jul 2005	Studied computational physics, including DFT and application to nano-structures at Brookhaven National Laboratory. Continued collaboration through 2008.
2003–2004 & 2005–2008	Teaching Assistant, Dept. of Physics, University of Utah Courses included physics for scientists and engineers, honors introductory physics, graduate statistical mechanics.
Skills	Experience with various DFT codes: Quantum-espresso, Profess, etc, including making modifications to them. Utilization, development and extension of legacy codes (mostly Fortran). From scratch code development for *ab initio* wave-function, DFT, and other calculations. Programming: C, C++, Fortran languages utilizing MPI. Scripting: BASH and others.

Publications

Ionic Transport Coefficients of Dense Plasmas without Molecular Dynamics,
J. Daligault, S.D. Baalrud, C.E. Starrett, D. Saumon, and T. Sjostrom, *Phys. Rev. Lett.* 116, 075002 (2016).

Ionic and electronic transport properties in warm dense matter by orbital-free density functional theory,
T. Sjostrom and J. Daligault, *Phys. Rev. E* 92, 063304 (2015).

A Liquid Regime Equation of State for Silicon Dioxide,
T. Sjostrom and S. Crockett, *SCCM 2015 Proceedings* (accepted).

Orbital-free extension to Kohn-Sham density functional theory equation of state calculations: Application to silicon dioxide,
T. Sjostrom and S. Crockett, *Phys. Rev. B* 92, 115104 (2015).

Gradient corrections to the exchange-correlation free energy,
T. Sjostrom and J. Daligault, *Phys. Rev. B* 90, 155109 (2014).

Fast and accurate quantum molecular dynamics of dense plasmas across temperature regimes,
T. Sjostrom and J. Daligault, *Phys. Rev. Lett.* 113, 155006 (2014).

Finite-temperature orbital-free DFT molecular dynamics: coupling Profess and Quantum Espresso,
V.V. Karasiev, T. Sjostrom, and S.B. Trickey, *Comput. Phys. Commun.* 185, 3240 (2014).

Accurate homogeneous electron gas exchange-correlation free energy for local spin-density calculations,
V.V. Karasiev, T. Sjostrom, J.Dufty, and S.B. Trickey, *Phys. Rev. Lett.* 112, 076403 (2014).

Nonlocal orbital-free noninteracting free-energy functional for warm dense matter,
T. Sjostrom and J. Daligault, *Phys. Rev. B* 88, 195103 (2013).

Uniform electron gas at finite temperatures,
T. Sjostrom and J. Dufty, *Phys. Rev. B* 88, 115123 (2013).

Innovations in Finite-Temperature Density Functionals,
V.V. Karasiev, T. Sjostrom, D.Chakraborty, J.W. Dufty, F.E. Harris, K. Runge, and S.B. Trickey, chapter in *Frontiers and Challenges in Warm Dense Matter*, Lecture Notes in Computational Science and Engineering, Vol. 96, F. Graziani et al. eds., (Springer 2014).

Generalized Gradient Approximation Non-interacting Free Energy Functionals for Orbital-free Density Functional Calculations,
V.V. Karasiev, T. Sjostrom, and S.B. Trickey, *Phys. Rev. B* 86, 115101 (2012).

Comparison of Density Functional approximations and the Finite-temperature Hartree-Fock Approximation in Warm Dense Lithium,
V.V. Karasiev, T. Sjostrom, and S.B. Trickey, *Phys. Rev. E* 86, 056704 (2012).

Temperature-Dependent Behavior of Confined Many-electron Systems in the Hartree-Fock Approximation,
T. Sjostrom, F.E. Harris, and S.B. Trickey, *Phys. Rev. B* 85, 045125 (2012).

Electronic Properties of Thin Film Periodic Nanostructures,
T. Sjostrom, D.C. Mattis, W.-G. Yin and W. Ku, *J. Comput. Theor. Nanosci.* Vol. 6, pp 403-417 (2009).

Electronic Energy Band Calculations in Nano-structures,
T. Sjostrom, Thesis, University of Utah (2008).

Bloch's Theorem in Nanoarchitectures,
D.C. Mattis and T. Sjostrom, *Mod. Phys. Lett. B,* Vol. 20, pp 501-513 (2006).

Presentations

APS-SCCM 2015 *Tampa*
A liquid regime equation of state for silicon dioxide, T. Sjostrom and S. Crockett.

APS March Meeting 2015 *San Antonio*
Self-diffusion and viscosity for warm dense systems by orbital-free density functional theory, T. Sjostrom and J. Daligault.

SCCS 2014 *Santa Fe*
Gradient corrections to the exchange-correlation free energy, T. Sjostrom and J. Daligault.

APS March Meeting 2014 *Denver*
Nonlocal orbital-free density functional theory for warm dense matter, T. Sjostrom and J. Daligault.

54th Sanibel Symposium, Feb. 2014 (Invited)
Nonlocal orbital-free density functional theory for warm dense matter.

APS-SCCM 2013 *Seattle*
Finite temperature orbital-free density functional theory MD for warm dense matter systems, T. Sjostrom and J. Daligault.

APS March Meeting 2013 *Baltimore*
Gradient corrections to finite-temperature exchange-correlation functionals, T. Sjostrom and J.W. Dufty.

14th Int'l Conf. on the Physics of Non-ideal Plasmas (PNP), Sept. 2012 (Poster) *Rostock*
Finite temperature Hartree-Fock and density functional theory calculations on confined hydrogen systems.

CECAM workshop: Orbital-free approach for high energy density physics, Sept. 2012 (Invited) *Paris*
Exchange-Correlation free energy functionals.

IPAM Computational Methods in High Energy Density Plasmas, Workshop IV: Computational Challenges in Warm Dense Matter, May 2012 (Invited) *UCLA*
Finite-Temperature Hartree-Fock Exchange and Exchange-Correlation Free Energy Functionals.

APS March Meeting 2012 *Boston*
Comparison of Finite Temperature Hartree-Fock and Density Functional Theory for Confined Systems, T. Sjostrom, S.B. Trickey, F.E. Harris.

APS DPP 2011 *Salt Lake City*
Temperature-Dependent Behavior of Confined Many-electron Systems in the Hartree-Fock Approximation, T. Sjostrom, F.E. Harris, S.B. Trickey.

APS March Meeting 2011 *Dallas*
Finite-temperature Exchange and Correlation Functionals in Self-Consistent Calculations, T. Sjostrom, V.V. Karasiev, S.B. Trickey.